

ABSTRACT

A quantum limit catalyst. The quantum limit corresponds to a size domain in which material properties are no longer constrained by the structure and bonding requirements imposed by the macroscopic length scale. The instant quantum limit catalyst is comprised of atomic aggregations
5 whose dimensions correspond to the quantum limit. In the quantum limit, the atomic aggregations acquire structural configurations and electronic interactions not attainable in the macroscopic limit. The structural configurations possible in the quantum limit correspond to atomic aggregations having bond lengths, bond angles, topologies and coordination environments that differ from those found in the macroscopic limit. The electronic interactions
10 possible in the quantum limit originate from wavefunction overlap and tunneling between atoms and lead to modifications in the magnitude and/or spatial distribution of electron density at catalytic sites to provide improved catalytic properties. The modifications in electron density and wavefunction characteristics (overlap and directionality) achieved in the quantum limit provide, in effect, “new” or “virtual” chemical elements whose structure and bonding deviate from those
15 associated with the “standard” chemical elements of conventional materials. Combinations of virtual elements provide virtual alloys having structures and properties not available in conventional alloys.

Representative quantum limit catalysts include materials comprised of quantum scale atomic aggregations of metal atoms. The aggregations include one or more metals and have sizes in the
20 angstrom scale range. Examples including catalysts derived from Fe, Mg, V and Co are disclosed. Catalytic properties are exemplified in the context of hydrogen storage. Methods that may be used to prepare quantum limit catalysts include sonochemical synthesis, thermal decomposition, and reduction.